



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:28 AM GMT

PDB ID : 2X78
Title : Human foamy virus integrase - catalytic core.
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Deposited on : 2010-02-24
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

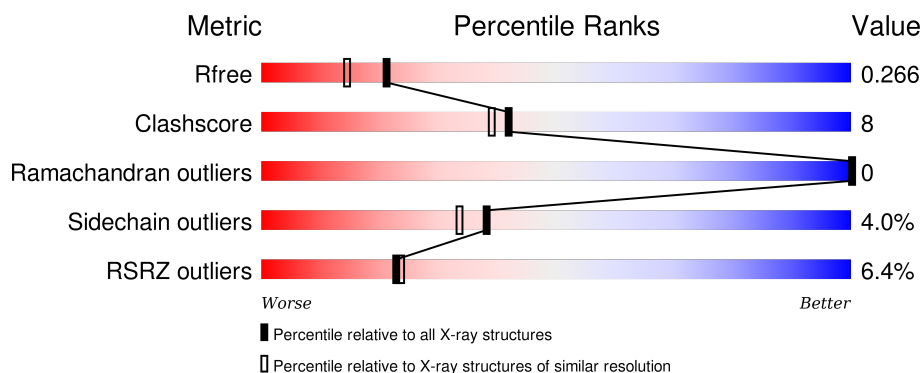
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	200	<div> <div>6%</div> <div>69% 15% • 15%</div> </div>
1	B	200	<div> <div>5%</div> <div>74% 13% • 12%</div> </div>
1	C	200	<div> <div>7%</div> <div>76% 15% • 9%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4626 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called INTEGRASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	171	Total	C	N	O	S	0	2	0
			1380	900	228	251	1			
1	B	176	Total	C	N	O	S	0	1	0
			1416	925	233	257	1			
1	C	183	Total	C	N	O	S	0	3	0
			1468	951	245	271	1			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	180	ARG	LYS	SEE REMARK 999	UNP P14350
B	180	ARG	LYS	SEE REMARK 999	UNP P14350
C	180	ARG	LYS	SEE REMARK 999	UNP P14350

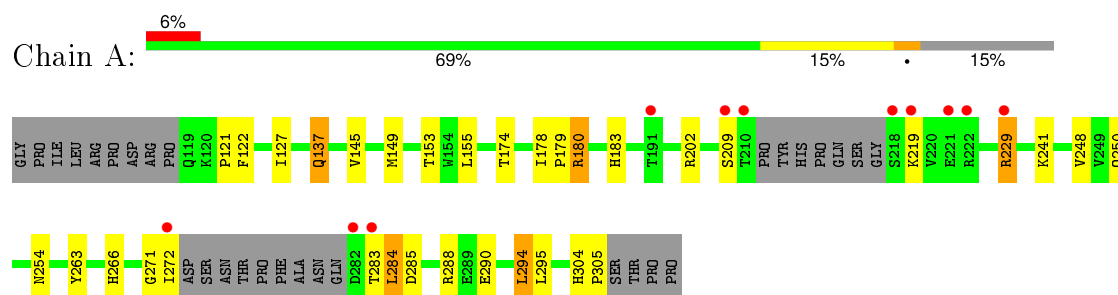
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	105	Total	O	0	0
			105	105		
2	B	110	Total	O	0	0
			110	110		
2	C	147	Total	O	0	0
			147	147		

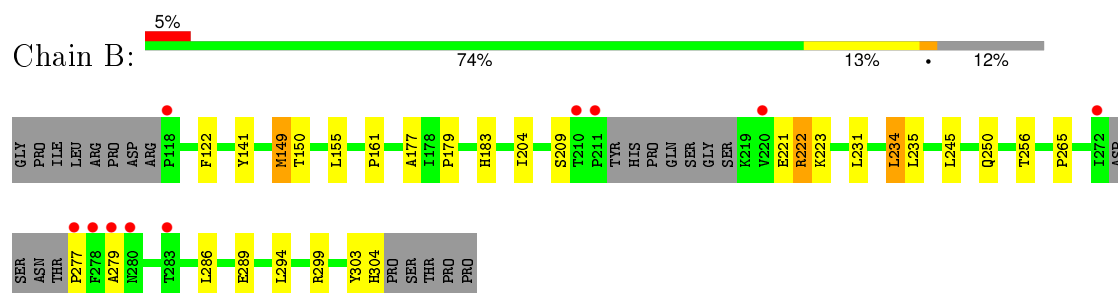
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

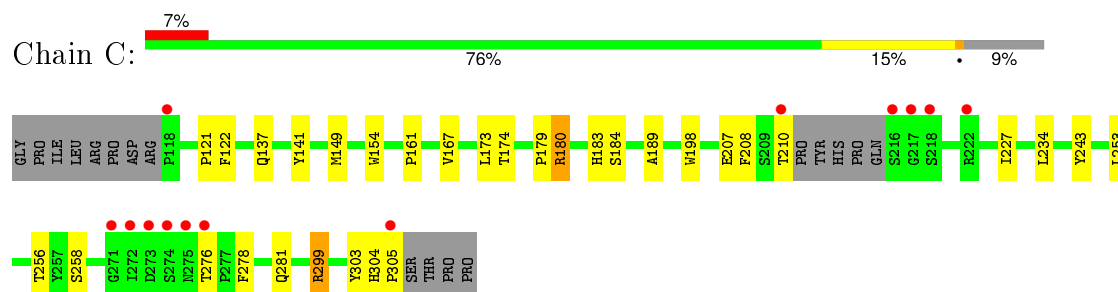
• Molecule 1: INTEGRASE



• Molecule 1: INTEGRASE



• Molecule 1: INTEGRASE



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	51.80 Å 98.04 Å 240.32 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.02 – 2.00 49.02 – 2.00	Depositor EDS
% Data completeness (in resolution range)	91.1 (49.02-2.00) 91.1 (49.02-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 2.00 Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.212 , 0.272 0.208 , 0.266	Depositor DCC
R_{free} test set	2113 reflections (5.83%)	DCC
Wilson B-factor (Å ²)	33.4	Xtriage
Anisotropy	0.219	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 52.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 38181 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4626	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.88% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.56	0/1427	0.58	0/1941
1	B	0.56	0/1458	0.57	1/1986 (0.1%)
1	C	0.62	0/1528	0.61	0/2080
All	All	0.58	0/4413	0.59	1/6007 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	234	LEU	CA-CB-CG	5.75	128.52	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1380	0	1401	28	0
1	B	1416	0	1432	20	0
1	C	1468	0	1472	28	0
2	A	105	0	0	3	0
2	B	110	0	0	5	0
2	C	147	0	0	2	0
All	All	4626	0	4305	72	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 8.

All (72) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202[B]:ARG:HH11	1:A:202[B]:ARG:HG2	0.90	1.04
1:A:202[B]:ARG:CG	1:A:202[B]:ARG:HH11	1.71	1.03
1:A:202[B]:ARG:NH1	1:A:202[B]:ARG:HG2	1.68	0.93
1:A:153:THR:H	1:A:254:ASN:HD21	1.22	0.87
1:A:229:ARG:HE	1:A:229:ARG:HA	1.44	0.83
1:A:284:LEU:HG	1:A:295:LEU:HD21	1.64	0.80
1:C:276:THR:HG21	1:C:278:PHE:HD2	1.55	0.72
1:C:304:HIS:HB2	1:C:305:PRO:HD3	1.71	0.72
1:B:155:LEU:H	1:B:250:GLN:NE2	1.88	0.71
1:C:276:THR:CG2	1:C:278:PHE:CD2	2.76	0.68
1:C:276:THR:HG21	1:C:278:PHE:CD2	2.28	0.67
1:C:304:HIS:CB	1:C:305:PRO:HD3	2.25	0.66
1:B:277:PRO:HD3	2:B:2091:HOH:O	1.99	0.62
1:C:122:PHE:O	1:C:179:PRO:HA	2.00	0.61
1:B:221:GLU:HB2	1:B:222:ARG:HE	1.65	0.61
1:C:243:TYR:OH	2:C:2114:HOH:O	2.17	0.60
1:C:180:ARG:HD3	1:C:180:ARG:N	2.17	0.59
1:A:266:HIS:HD2	2:B:2033:HOH:O	1.84	0.59
1:A:241:LYS:NZ	1:A:290:GLU:HG3	2.18	0.59
1:C:304:HIS:HB2	1:C:305:PRO:CD	2.33	0.58
1:A:202[B]:ARG:CG	1:A:202[B]:ARG:NH1	2.43	0.57
1:C:299[B]:ARG:NH2	2:C:2129:HOH:O	2.37	0.57
1:C:174:THR:HG22	1:C:179:PRO:HD3	1.86	0.56
1:C:276:THR:HG22	1:C:278:PHE:H	1.71	0.56
1:B:304:HIS:HE1	1:C:141:TYR:OH	1.89	0.55
1:A:178:ILE:CD1	1:B:286:LEU:HD23	2.37	0.55
1:A:271:GLY:HA2	2:A:2091:HOH:O	2.06	0.54
1:A:174:THR:HG22	1:A:179:PRO:HD3	1.90	0.53
1:C:304:HIS:CB	1:C:305:PRO:CD	2.87	0.52
1:B:149:MET:HG3	1:B:150:THR:N	2.20	0.52
1:C:161:PRO:O	1:C:189:ALA:HB2	2.09	0.52
1:C:121:PRO:O	1:C:122:PHE:HB2	2.10	0.51
1:C:234:LEU:HD23	1:C:234:LEU:O	2.10	0.50
1:A:155:LEU:H	1:A:250:GLN:NE2	2.09	0.50
1:A:122:PHE:O	1:A:179:PRO:HA	2.12	0.50
1:B:265:PRO:HD3	2:B:2078:HOH:O	2.12	0.50
1:B:223:LYS:NZ	2:B:2058:HOH:O	2.43	0.49
1:B:183:HIS:CE1	1:B:209:SER:HB3	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:184:SER:O	1:C:208:PHE:HA	2.12	0.49
1:C:227:ILE:HG12	1:C:253:LEU:HD11	1.94	0.48
1:A:263:TYR:CE1	1:A:272:ILE:HG21	2.48	0.48
1:C:256:THR:HG23	1:C:303:TYR:CZ	2.48	0.48
1:A:229:ARG:NH2	2:A:2064:HOH:O	2.47	0.48
1:C:137:GLN:HG3	1:C:243:TYR:CD2	2.49	0.47
1:A:180:ARG:HD3	1:B:279:ALA:HB2	1.95	0.47
1:B:256:THR:HG23	1:B:303:TYR:CZ	2.49	0.47
1:B:122:PHE:CD2	1:B:177:ALA:HB3	2.50	0.47
1:A:137:GLN:HE21	1:A:137:GLN:N	2.13	0.46
1:B:299:ARG:NH1	2:B:2107:HOH:O	2.49	0.45
1:A:178:ILE:HD11	1:B:286:LEU:HD23	1.98	0.45
1:A:153:THR:H	1:A:254:ASN:ND2	2.03	0.45
1:C:183:HIS:ND1	1:C:207:GLU:HG3	2.31	0.45
1:A:304:HIS:HA	1:A:305:PRO:HD2	1.85	0.43
1:A:241:LYS:HZ2	1:A:290:GLU:HG3	1.84	0.43
1:B:245:LEU:HB3	1:B:294:LEU:CD2	2.50	0.42
1:A:248:VAL:HG12	1:A:294:LEU:HD23	2.02	0.42
1:B:155:LEU:H	1:B:250:GLN:HE21	1.62	0.42
1:B:179:PRO:O	1:B:204:ILE:HG12	2.20	0.42
1:B:231:LEU:O	1:B:235:LEU:HG	2.19	0.42
1:B:141:TYR:CE1	1:B:161:PRO:HD3	2.54	0.41
1:A:241:LYS:HZ3	1:A:290:GLU:HG3	1.84	0.41
1:A:183:HIS:CE1	1:A:209:SER:HB3	2.55	0.41
1:A:283:THR:HG21	2:A:2077:HOH:O	2.20	0.41
1:C:167:VAL:HG13	1:C:198:TRP:CD1	2.56	0.41
1:A:121:PRO:O	1:A:122:PHE:HB2	2.21	0.41
1:B:122:PHE:O	1:B:179:PRO:HA	2.21	0.41
1:A:127:ILE:HG22	1:A:145:VAL:HG22	2.02	0.41
1:C:154:TRP:CE2	1:C:173:LEU:HD11	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	167/200 (84%)	162 (97%)	5 (3%)	0	100	100
1	B	171/200 (86%)	166 (97%)	5 (3%)	0	100	100
1	C	182/200 (91%)	174 (96%)	8 (4%)	0	100	100
All	All	520/600 (87%)	502 (96%)	18 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	157/181 (87%)	148 (94%)	9 (6%)	25	19
1	B	159/181 (88%)	155 (98%)	4 (2%)	55	55
1	C	168/181 (93%)	161 (96%)	7 (4%)	36	31
All	All	484/543 (89%)	464 (96%)	20 (4%)	38	32

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	137	GLN
1	A	149	MET
1	A	180	ARG
1	A	219	LYS
1	A	229	ARG
1	A	284	LEU
1	A	285	ASP
1	A	288	ARG
1	A	294	LEU
1	B	149	MET
1	B	222	ARG
1	B	234	LEU
1	B	289	GLU

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Mol	Chain	Res	Type
1	C	149	MET
1	C	180	ARG
1	C	210	THR
1	C	258	SER
1	C	281	GLN
1	C	299[A]	ARG
1	C	299[B]	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	137	GLN
1	A	250	GLN
1	A	254	ASN
1	A	266	HIS
1	B	250	GLN
1	B	266	HIS
1	B	281	GLN
1	B	304	HIS
1	C	255	ASN
1	C	281	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	171/200 (85%)	0.49	11 (6%) 23 24	22, 36, 65, 87	1 (0%)
1	B	176/200 (88%)	0.49	10 (5%) 27 29	20, 34, 65, 71	0
1	C	183/200 (91%)	0.40	13 (7%) 19 20	14, 28, 61, 74	0
All	All	530/600 (88%)	0.46	34 (6%) 23 24	14, 32, 65, 87	1 (0%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	210	THR	5.3
1	C	210	THR	4.9
1	B	210	THR	4.8
1	C	216	SER	4.6
1	A	218	SER	4.4
1	C	274	SER	4.3
1	A	219	LYS	4.3
1	C	218	SER	4.1
1	A	222	ARG	4.1
1	C	275	ASN	4.0
1	A	282	ASP	4.0
1	C	272	ILE	3.5
1	A	209	SER	3.4
1	B	279	ALA	3.3
1	C	217	GLY	3.3
1	B	283	THR	3.2
1	A	283	THR	3.0
1	B	277	PRO	2.9
1	B	278	PHE	2.9
1	B	220	VAL	2.9
1	C	305	PRO	2.9
1	B	211	PRO	2.9
1	B	118	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	222	ARG	2.8
1	A	272	ILE	2.6
1	B	280	ASN	2.6
1	A	191	THR	2.5
1	C	273	ASP	2.4
1	C	118	PRO	2.4
1	A	221	GLU	2.2
1	A	229	ARG	2.2
1	C	276	THR	2.2
1	B	272	ILE	2.1
1	C	271	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.